Predicting Metabolic Stability of Drug Molecules

ABSTRACT OF THE DISCLOSURE

Methods are disclosed for developing models used to rapidly predict metabolic stability and regioselectivity of drug molecules. Training sets, based on a sample of molecules with known reaction rates and/or activation energies, are used along with structural descriptors of the molecules in order to develop mathematical models of metabolism based on regression analysis of the activation energies and descriptors. The resulting models are then used to predict the metabolism of other molecules. The invention is particularly useful in developing simple models of cytochrome p450 enzyme metabolism.